Chapter 16

Numerical Integration Formulas

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Chapter Objectives

- Understanding Newton-Cotes integration formulas which based on the strategy of replacing a complicated or tubulated data with a polynomial.
- Knowing how to implement the following single application Newton-Cotes formulas: Trapezoidal rule, Simpson’s 1/3 rule, Simpson’s 3/8 rule
- Knowing how to implement the following composite Newton-Cotes formulas: Trapezoidal rule, Simpson’s 1/3 rule,
- Recognizing that even-segment-odd-point formulas like Simpson’s 1/3 rule achieve higher than expected accuracy.
- Understanding the difference between open and closed integration formulas.

YOU’VE GOT A PROBLEM

The velocity of free-falling bungee jumper as a function of time is

\[ v(t) = \sqrt{\frac{g m}{c_d}} \tanh \left( \sqrt{\frac{g c_d}{m}} t \right) \]

So the vertical distance \( z \) the jumper has fallen after a certain time \( t \) is

\[ z(t) = \int_0^t v(t) \, dt \]

or

\[ z(t) = \int_0^t \sqrt{\frac{2 g m}{c_d}} \tanh \left( \sqrt{\frac{g c_d}{m}} t \right) \, dt \] \hspace{1cm} (1)

or

\[ z(t) = \frac{m}{c_d} \ln \left[ \cosh \left( \sqrt{\frac{g c_d}{m}} t \right) \right] \]

we have analytic solution in this case.

Some Reasons for needing numerical integration.

1. But there are other functions that cannot be integrated analytically.
2. There are velocities along with their associated times could be assembled as a table of discrete values. In this situation, it would also be possible to integrate the discrete data to determine the distance.
**INTRODUCTION AND BACKGROUND**

*What is Integration?*

\[ I = \int_{a}^{b} f(x)dx \]

is the total value, or summation, of \( f(x)dx \) over the range \( x = a \) to \( b \). For functions lying above the \( x \) axis, the integral corresponds to the area under the curve of \( f(x) \) between \( x = a \) and \( b \).

*Integration in Engineering and Science*

Mean

\[ \text{Mean} = \frac{\sum_{i=1}^{n} y_i}{n} : \text{discrete case} \]

\[ \text{Mean} = \frac{\int_{a}^{b} f(x)dx}{b-a} : \text{continuous case} \]

Integrals are also employed by engineers and scientists to evaluate the total amount or quantity of a given physical variable.

For example:

\[ \text{Mass} = \text{concentration} \times \text{volume} \]

If the concentration varies from location to location, it is necessary to sum the products of local concentrations \( c_i \) and corresponding elemental volumes \( \Delta V_i \):

\[ \text{Mass} = \sum_{i=1}^{n} c_i \Delta V_i : \text{discrete case} \]

where \( n \) is the number of discrete volumes.

\[ \text{Mean} = \iiint c(x, y, z)dx dy dz : \text{continuous case} \]

or

\[ \text{Mean} = \iiint_{V} c(V)dV \]

where \( c(x, y, z) \) is a known concentration function and \( x, y, \) and \( z \) are independent variables designating position in Cartesian coordinates.

The total rate of energy transfer across a plane where the flux(rate of energy per unit area) is a function of position is given by

\[ \text{Flux} = \iint_{A} \text{flux} \, dA \]
NEWTON-COTES FORMULAS

The Newton-Cotes formulas are based on the strategy of replacing a complicated function or tabulated data with a polynomial that is easy to integrate:

\[ I = \int_a^b f(x) \, dx \approx \int_a^b f_n(x) \, dx \]  \hspace{1cm} (2)

where \( f_n(x) \) = a polynomial of the form

\[ f_n(x) = a_0 + a_1 x + \cdots + a_{n-1} x^{n-1} + a_n x^n \]

A first-order polynomial is used as an approximation(left). A parabola is used for same purpose(right).
A series of polynomials applied piecewise can be used. The Figure shows that a three straight segments are used.

Closed form: the beginning and end of the limits of integration are known. Open form: they are not known. We emphasizes the closed form.

**THE TRAPEZOIDAL RULE**
The first of the Newton-Cotes closed integral formulas. The polynomial in Equation 2 is first-order:

\[
I = \int_a^b \left[ f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx
\]  \hspace{1cm} (3)

The result of the integration is

\[
I = (b - a) \frac{f(a) + f(b)}{2}
\]  \hspace{1cm} (4)

which is called the trapezoidal rule. The trapezoidal rule is equivalent to approximating the area of the trapezoid under the straight line connecting \( f(a) \) and \( f(b) \) in Figure 16.7. So

\[
I = \text{width} \times \text{average height} = (b - a) \times \text{average height} = (b - a) \frac{f(a) + f(b)}{2}
\]  \hspace{1cm} (5)

**Error of the Trapezoidal Rule**
The error (See Figure 16.8) of the trapezoidal rule is

\[
E_t = -\frac{1}{12} f''(\xi)(b - a)^3
\]  \hspace{1cm} (6)
where \( \xi \) lies somewhere in the interval from \( a \) to \( b \).

If a function is linear \( E_i = 0 \).

\[ \text{Example 0.1} \quad \text{Use Equation 4 to numerically integrate} \]

\[ f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 \]

from \( a = 0 \) to \( b = 0.8 \). The exact value is 1.640533.

\[ \text{Solution} \]
Since \( f(0) = 0.2 \) and \( f(0.8) = 0.232 \) we have
\[
I = (0.8 - 0) \frac{0.2 + 0.232}{2} = 0.1728
\]
And error is
\[
E_t = 1.640533 - 0.1728 = 1.467723
\]
which corresponds to a percent relative error of \( \varepsilon_t = 89.5\% \). Too Big (See Figure 16.8).

On the other hand, using Equation 6 we have
\[
E_a = -\frac{1}{12}(-60)(0.8)^3 = 2.56
\]
where
\[
f''(x) = -400 + 4,050x - 10,800x^2 + 8,000x^3
\]
and the average value (not accurate) of the second derivative is
\[
\bar{f}''(x) = \frac{\int_0^{0.8} (-400 + 4,050x - 10,800x^2 + 8,000x^3) \, dx}{0.8 - 0} = -60
\]
No difference!!

**The Composite Trapezoidal Rule**

Divide the integral interval from \( a \) to \( b \) into a number of segments and apply
the trapezoidal rule (See Figure 16.9). And add the results.

\((a = x_0, x_1, x_2, \ldots, b = x_n) : (n - 1)\) equally spaced base points \}

So width of the segments is
\[
h = \frac{b - a}{n} \quad (7)
\]
The total integral can be represented as
\[
I = \int_{x_0}^{x_1} f(x) \, dx + \int_{x_1}^{x_2} f(x) \, dx + \cdots + \int_{x_{n-1}}^{x_n} f(x) \, dx
\]
Substitute the trapezoidal rule for each interval yields
\[
I = h \frac{f(x_0) + f(x_1)}{2} + h \frac{f(x_1) + f(x_2)}{2} + \cdots + h \frac{f(x_{n-1}) + f(x_n)}{2} \quad (8)
\]
or
\[
I = \frac{h}{2} \left[ f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right] \quad (9)
\]
or, by Equation 7,

\[ I = \frac{b - a}{\text{width}} \left( f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right) \frac{2}{n} \text{Average height} \]  

(10)

An error for the composite trapezoidal rule can be obtained by summing the individual errors for each segment to give

\[ E_t = -\frac{(b - a)^3}{12n^3} \sum_{i=1}^{n} f''(\xi_i) \]  

(11)

where \( f''(\xi_i) \) is the second derivative at a point \( \xi_i \) located in segment \( i \).

Let the average value of the second derivative for the entire interval as

\[ f'' \approx \frac{\sum_{i=1}^{n} f''(\xi_i)}{n} \]

Then an approximate error is

\[ E_a = -\frac{(b - a)^3}{12n^2} f'' \]

Thus, if the number of segments is doubled, the truncation error will be quartered.

| TABLE 16.1 | Results for the composite trapezoidal rule to estimate the integral of \( f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 \) from \( x = 0 \) to \( 8 \). The exact value is 1.640533. |
|---|---|---|---|---|
| \( n \) | \( h \) | \( I \) | \( e_i (\%) \) |
| 2 | 0.4 | 1.0688 | 34.9 |
| 3 | 0.2667 | 1.3695 | 16.5 |
| 4 | 0.2 | 1.4848 | 9.5 |
| 5 | 0.16 | 1.5399 | 6.1 |
| 6 | 0.1333 | 1.5703 | 4.3 |
| 7 | 0.1143 | 1.5887 | 3.2 |
| 8 | 0.1 | 1.6008 | 2.4 |
| 9 | 0.0889 | 1.6091 | 1.9 |
| 10 | 0.08 | 1.6150 | 1.6 |

그림 1: Summary of Errors of the trapezoidal rule.

**Example 0.2** Use two-segment trapezoidal rule to estimate the integral of

\[ f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 \]

from \( a = 0 \) to \( b = 0.8 \). The exact value is 1.640533.
Solution

For \( n = 2(h = 0.4) \):

\[
\begin{align*}
  f(0) &= 0.2 & f(0.4) &= 2.456 & f(0.8) &= 0.232 \\
  I &= 0.8 \frac{0.2 + 2(2.456) + 0.232}{4} = 1.0688 \\
  E_t &= 1.640533 - 1.0688 = 0.57173 & \varepsilon_t &= 34.9\% \\
  E_n &= -\frac{0.8^3}{12(2)^2}(-60) = 0.64 \\
\end{align*}
\]

where \(-60\) is the average second derivative determined previously.

**MATLAB M-file: trap**

A simple algorithm to implement the composite trapezoidal rule:

```matlab
function I = trap(func, a, b, n)
% trap(func, a, b, n):
% composite trapezoidal rule.
% input:
% func = name of function to be integrated
% a, b = integration limits
% n = number of segments
% output:
% I = integral estimate

x = a;
for j = 1 : n-1
    x = x + h;
    s = s + 2*feval(func, x);
end
s = s + feval(func,b);
I = (b-a)* s/(2*n);
```
Example 0.3  By evaluating the integral of Equation 1, determine the distance fallen by the free-falling bungee jumper in the first 3 seconds. The exact value of the integral is 41.94805.

Solution

\[ g = 9.81 \text{m/s}^2, \quad m = 68.1 \text{kg}, \quad \text{and} \quad c_d = 0.25 \text{kg/m} \]

\[
\begin{align*}
\gg v &= \text{inline}('\sqrt{9.81*68.1/0.25}... \\
& \quad \tanh(\sqrt{9.81*0.25/68.1}*t)') \\
\end{align*}
\]

\[ v = \]

Inline function:

\[ v(t) = \sqrt{9.81*68.1/0.25}... \\
& \quad \tanh(\sqrt{9.81*0.25/68.1}*t) \]

\[
\begin{align*}
\gg \text{format long} \\
\gg \text{trap}(v,0,3,5) \\
\text{ans} &= \\
41.86992959072735 \\
\gg \text{trap}(v,0,3,10000) \\
\text{x} &= \\
41.948049999917528
\end{align*}
\]

SIMPSON’S RULES

We use higher-order polynomials such as a parabola (See Figure 16.11(a)) or a third-order polynomial (See Figure 16.11(b)). The formulas that result from taking the integral under these polynomials are called Simpson’s rules.

Simpson’s 1/3 Rule

Simpson’s 1/3 rule corresponds to the case where the polynomial in Equation 2 is second-order:

\[
\begin{align*}
I &= \int_{x_0}^{x_2} \left[ \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \\
& \quad + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \right] dx \\
\end{align*}
\]

where \(a\) and \(b\) are designated as \(x_0\) and \(x_2\), respectively. The result is

\[
I = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] : \text{Simpson’s 1/3 rule}
\]
or
\[ I = (b - a) \frac{f(x_0) + 4f(x_1) + f(x_2)}{6} \]  
(14)

where \( h = (b - a)/2 \).

Error (known)
\[ E_t = -\frac{1}{90} h^5 f^{(4)}(\xi) \]
or, because \( h = (b - a)/2 \):
\[ E_t = -\frac{(b - a)^5}{2880} f^{(4)}(\xi) \]  
(15)

where \( \xi \) lies somewhere in the interval \([a, b]\). If a given polynomial is cubic, then the error is 0. It yields exact results for cubic polynomials even though it is derived from a parabola!

\textbf{Example 0.4}  
Use Equation 14 to integrate
\[ f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 \]
from \( a = 0 \) to \( b = 0.8 \). Employ Equation 15 to estimate the error. The exact value is 1.640533.

\textbf{Solution}  
For \( n = 2 \) (\( h = 0.4 \)):
\[ f(0) = 0.2 \quad f(0.4) = 2.456 \quad f(0.8) = 0.232 \]
\[ I = 0.8 \frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467 \]

\[ E_t = 1.640533 - 1.367467 = 0.2730667 \quad \varepsilon_t = 16.6\% \quad (16) \]

\[ E_a = -\frac{0.85}{2880}(-2400) = 0.2730667 \]

where \(-2400\) is the average fourth derivative. Five time more accurate than for a single application of the trapezoidal rule.

**The Composite Simpson’s 1/3 Rule**

divide the integration interval into a number of segments of equal width. (See Figure 16.12) The total integral is:

\[ I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx \quad (17) \]

Substitute Simpson’s 1/3 rule for each integral yields

\[ I = \frac{2h}{6} f(x_0) + 4f(x_1) + 2h f(x_2) + 4f(x_3) + f(x_4) \]

\[ + \cdots + \frac{2h}{6} f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \quad (18) \]

or,

\[ I = (b - a) \frac{f(x_0) + 4 \sum_{i=1,3,5} f(x_i) + 2 \sum_{j=2,4,6} f(x_j) + f(x_n)}{3n} \quad (19) \]
where \( n \) is even(REQUIRED!!).

An error estimate

\[
E_a = -\frac{(b - a)^5}{180n^4} f^{(4)}
\]  

(20)

♦ Example 0.5 Use Equation 19 with \( n = 4 \) to estimate the integral of

\[
f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5
\]

from \( a = 0 \) to \( b = 0.8 \). Employ Equation 20 to estimate the error. The exact value is 1.640533.

Solution

For \( n = 4(h = 0.2) \):

\[
\begin{align*}
f(0) &= 0.2 & f(0.2) &= 1.288 \\
f(0.4) &= 2.456 & f(0.6) &= 3.464 \\
f(0.8) &= 0.232
\end{align*}
\]

\[
I = 0.8 \frac{0.2 + 4(1.288 + 3.464) + 2(0.456) + 0.232}{12} = 1.623467
\]  

(21)

\[
E_t = 1.640533 - 1.623467 = 0.017067 \\ \epsilon_t = 1.04\%
\]

\[
E_a = -\frac{0.8^5}{180(4)^4}(-2400) = 0.017067
\]

Note \( E_t = E_a \).

Restriction : even number of segments and equispaced. Then What? What?

What?

The Simpson’s 3/8 Rule

A third order Lagrange polynomial can be fit to four points and integrated to yield

\[
I = \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] : \text{Simpson’s 3/8 rule}
\]

where \( h = (b - a)/3 \). It is the third Newton-Cotes closed integration formula. Express it in the form of Equation 5:

\[
I = (b - a) \frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}
\]  

(22)

An errors:

\[
E_t = -\frac{3}{80} h^5 f^{(4)}(\xi)
\]
or, because \( h = (b - a)/3 \):

\[
E_I = -\frac{(b - a)^5}{6480} f^{(4)}(\xi)
\]  

(23)

Because the denominator of Equation 23 is larger than for Equation 15, the 3/8 rule is somewhat more accurate than the 1/3 rule.

When \( n \) is odd we combine the Simpson’s 1/3 rule and Simpson’s 3/8 rule, for example see Figure 16.13.

♦ Example 0.6  
(a) Use Simpson 3/8 rule to integrate

\[
f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5
\]

from \( a = 0 \) to \( b = 0.8 \).

(b) Use it in conjunction with Simpson’s 1/3 rule to integrate the same function for five segments. The exact value is 1.640533.

Solution

(a) Four equally spaced points are needed:

\[
f(0) = 0.2 \quad f(0.2667) = 1.432724
\]

\[
f(0.5333) = 3.487177 \quad f(0.8) = 0.232
\]

\[
I = 0.8 \frac{0.2 + 3(1.432724 + 3.487177) + 0.232}{8} = 1.51970
\]

(24)
(b) five equally spaced points are needed ($h = 0.16$):

\[
\begin{align*}
    f(0) &= 0.2 & f(0.16) &= 1.296929 \\
    f(0.32) &= 1.743393 & f(0.48) &= 3.186015 \\
    f(0.64) &= 3.181929 & f(0.80) &= 0.232
\end{align*}
\]  

(25)

Simpson’s 1/3 rule for the first two segments

\[
I_1 = 0.32 \frac{0.2 + 4(1.296919) + 1.743393}{6} = 0.3803237
\]

and for the last three segments, Simpson’s 3/8 rule used to obtain

\[
I_2 = 0.48 \frac{1.743393 + 3(3.186015 + 3.181929) + 0.232}{8} = 1.264754
\]

So

\[
I = I_1 + I_2 = 0.3803237 + 1.264754 = 1.645077
\]

**HIGHER-ORDER NEWTON-COTES FORMULAS**

Newton-Cotes closed integration formulas: trapezoidal rule and Simpson’s rule. Some of the formulas are summarized in Table 16.2. Simpson’s rules are sufficient for most applications.

**INTEGRATION WITH UNEQUAL SEGMENTS**

Unequal-sized segments.

\[
I = h_1 \frac{f(x_0) + f(x_1)}{2} + h_2 \frac{f(x_1) + f(x_2)}{2} + \cdots + h_n \frac{f(x_{n-1}) + f(x_n)}{2}
\]  

(26)
where $h_i =$ the width of segments $i$.

**Example 0.7  Trapezoidal Rule with Unequal Segments**

The information in Table 16.3 was generated using the same polynomial employed in Example 0.1. Use Equation 26 to determine the integral for this data. Recall that the correct answer is 1.640533.

**Solution**

$$I = 0.12 \frac{0.2 + 1.309729}{2} + 0.10 \frac{1.309729 + 1.305241}{2} + \cdots + 0.10 \frac{2.363 + 0.232}{2} = 1.594801$$

with an absolute percent relative error of $\varepsilon_t = 2.8\%$.

**MATLAB M-file : trapuneq**

A simple algorithm to implement the trapezoidal rule for unequally spaced data can be written as below.

rules for $x$ and $y$ in the algorithm.

1. The two vectors are of the same length.

2. The $x$’s are in ascending order.

3. subscripts in Equation 26 need to be modified to account for the fact that MATLAB does not allow zero subscripts in arrays.

The algorithm :

```matlab
function integr = trapuneq(x, y)
% trapuneq(x, y):
% Applies the trapezoidal rule to determine
% the integral for n data points (x,y)
%```
% where x must be in ascending order.
% input:
% x = independent variable
% y = dependent variable
% output:
% integr = integral

n = length(x);
if length(y) ~=n, error('x and y must be same ...
   length'); end
s = 0;
for i = 1 : n-1
   if x(i+1) < x(i)
       error('x values must be in descending order' );
   end
   s = s + (x(i+1) - x(i))*(y(i) + y(i+1))/2;
end
integr = s;

******************************

Execution:
>> x = [0 .12 .22 .32 .36 .4 .44 .54 .64 .7 .8];
>> y = 0.2 + 25*x - 200*x.^2 + 675*x.^3 - 900*x.^4 + 400*x.^5;
>> trapuneq(x,y)
ans =
1.5948
which is identical to the result obtained in Example 0.7.

MATLAB Function : trapz

Syntax :

z = trapz(x, y)

where the vectors, x and y, hold the independent and dependent variables, respectively.
>> x = [0 .12 .22 .32 .36 .4 .44 .54 .64 .7 .8];
>> y = 0.2 + 25*x - 200*x.^2 + 675*x.^3 - 900*x.^4 + 400*x.^5;
>> trapz(x,y)
  ans =
          1.5948

OPEN METHODS

Recall from Figure 16.6(b) that open integration formulas have limits that extend beyond the range of the data. Table 16.4 summarize the Newton-Cotes open integration formulas based on Equation 5 We will discuss it again in Chapter 18 and 19.

MULTIPLE INTEGRALS

A general equation to compute the average of a two-dimensional function can be written as

$$T = \frac{\int_{a}^{b} \left( \int_{c}^{d} f(x, y) \,dx \right) \,dy}{(d-c)(b-a)}$$  \hspace{1cm} (28)

The double integral of a function over a rectangular area(Figure 16.15)

♦ Example 0.8  Suppose that the temperature of a rectangular heated plate is described by the following function :

$$T(x, y) = 2xy + 2x - x^2 - 2y^2 + 40$$

If the plate is 8 m long(x dimension) and 6 m wide(y dimension), compute the average temperature.
**Solution** The correct answer is 58.66667. See Figure 16.16

The trapezoidal rule:

is implemented along $x$ dimension for each $y$ value. These values are then integrated along the $y$ dimension to give the final result of 2688. So $2688/(6 \times 8) = 56$ (How? HOMEWORK!!)

A single segment Simpson’s 1/3 rule:

$2816/(6 \times 8) = 58.66667$. (How? HOMEWORK!!) We have exact value because the given polynomial is quadratic. Note that Simpson’s 1/3 rule yielded perfect results for cubic polynomial.